4-Chlorobutyl m-tolyl ether

Other names: 1-(4-chlorobutoxy)-3-methylbenzene
Inchi: InChI=1S/C11H15ClO/c1-10-5-4-6-11(9-10)13-8-3-2-7-12/h4-6,9H,2-3,7-8H2,1H3
InchiKey: FVBUVUOPHWUVCR-UHFFFAOYSA-N
Formula: C11H15ClO
SMILES: Cc1cccc(OCCCCCl)c1
Mol. weight [g/mol]: 198.69
CAS: 71648-39-0

Physical Properties

Property code	Value	Unit	Source
gf	27.59	kJ/mol	Joback Method
hf	-193.27	kJ/mol	Joback Method
hfus	23.28	kJ/mol	Joback Method
hvap	49.81	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.393		Crippen Method
mcvol	160.200	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1522.80		NIST Webbook
rinpol	1522.80		NIST Webbook
tb	542.59	K	Joback Method
tc	749.09	K	Joback Method
tf	304.82	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.02	J/mol×K	542.59	Joback Method
cpg	369.55	J/mol×K	577.01	Joback Method
cpg	383.33	J/mol×K	611.42	Joback Method
cpg	396.37	J/mol×K	645.84	Joback Method
cpg	408.69	J/mol×K	680.26	Joback Method
cpg	420.31	J/mol×K	714.68	Joback Method

cpg	431.25	J/mol×K	749.09	Joback Method
dvisc	0.0018569	Pa×s	304.82	Joback Method
dvisc	0.0010069	Pa×s	344.45	Joback Method
dvisc	0.0006194	Pa×s	384.08	Joback Method
dvisc	0.0004173	Pa×s	423.70	Joback Method
dvisc	0.0003008	Pa×s	463.33	Joback Method
dvisc	0.0002283	Pa×s	502.96	Joback Method
dvisc	0.0001804	Pa×s	542.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71648390&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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